AFRL-RX-WP-TP-2011-4238

LARGE DATASET GENERATION, INTEGRATION AND SIMULATION IN MATERIALS SCIENCE (PREPRINT)

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JUNE 2011

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UNITED STATES AIR FORCE

REPORT DOCUMENTATION PAGE	*Form Approved* *OMB No. 0704-0188*

1. REPORT DATE *(DD-MM-YY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
June 2011	Journal Article Preprint	01 June 2011 – 01 June 2011

4. TITLE AND SUBTITLE

LARGE DATASET GENERATION, INTEGRATION AND SIMULATION IN MATERIALS SCIENCE (PREPRINT)

5a. CONTRACT NUMBER In-house

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER 62102F

6. AUTHOR(S)

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5d. PROJECT NUMBER 4347

5e. TASK NUMBER 20

5f. WORK UNIT NUMBER LM121100

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Metals Branch (AFRL/RXLM)
Metals, Ceramics, and NDE Division
Air Force Research Laboratory, Materials and Manufacturing Directorate
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Air Force Materiel Command, United States Air Force

The Ohio State University

8. PERFORMING ORGANIZATION REPORT NUMBER

AFRL-RX-WP-TP-2011-4238

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750
Air Force Materiel Command
United States Air Force

10. SPONSORING/MONITORING AGENCY ACRONYM(S)

AFRL/RXLM

11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)

AFRL-RX-WP-TP-2011-4238

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

PAO Case Number: 88ABW 2011-0256 Clearance Date: 24 Jan 2011. Document contains color.

Journal article submitted to the *Journal of Metals*.

14. ABSTRACT

As new and rapid materials characterization tools become widely available, large datasets are been generated at a faster and faster pace, which is both exciting and challenging. The exciting aspects are that large amounts of composition, structure, and spectral information about materials are being gathered routinely. This promises to accelerate the traditional scientific pursuits in Materials Science of establishing processing-structure and structure-property relationships and hypothesis testing. Even more exciting is the promise to provide quantitative validations of the physics-based forward models of these input-response relationships by providing statistically significant datasets for this validation. The main challenges presented by the emergence of these techniques are (1) rapid acquisition of larger and larger datasets, (2) using this information to provide predictive capabilities in materials systems, and (3) analysis of the increasing volumes of data.

15. SUBJECT TERMS

integration, simulation, data generation

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT:	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON (Monitor)
a. REPORT	b. ABSTRACT	c. THIS PAGE			
Unclassified	Unclassified	Unclassified	SAR	8	Jeff Simmons
					19b. TELEPHONE NUMBER *(Include Area Code)* N/A

Large Dataset Generation, Integration and Simulation in Materials Science

Jeff Simmons and J.-C. Zhao

As new and rapid materials characterization tools become widely available, large datasets are been generated at a faster and faster pace, which is both exciting and challenging. The exciting aspects are that large amounts of composition, structure, and spectral information about materials are being gathered routinely. This promises to accelerate the traditional scientific pursuits in Materials Science of establishing processing-structure and structure-property relationships and hypothesis testing. Even more exciting is the promise to provide quantitative validations of the physics-based forward models of these input-response relationships by providing statistically significant datasets for this validation. The main challenges presented by the emergence of these techniques are (1) rapid acquisition of larger and larger datasets, (2) using this information to provide predictive capabilities in materials systems, and (3) analysis of the increasing volumes of data. The selected articles highlighted here provide a snapshot of some current activities in this expanding field, but, in no way, attempt to cover the entire field-such an attempt would be well beyond the page limit of a JOM issue.

Four articles were chosen to highlight data generation. The article by Uchic, Groeber, and Rollett describes the current state of the art of automated serial sectioning. That by Barabash, Bei, Ice, Gao, and Barabash describes one of the exciting developments in X-ray characterization: that of characterization of internal strains in materials. The article by Kotula and Sorensen describes recent advances in hyperspectral X-ray materials characterization and some techniques used to fuse the signals from multiple wavelengths into a single coherent picture of material structure. J.-C. Zhao and D. Cahill describe recent development of femtosecond-laser based measurements of thermal conductivity, expansion coefficients and elastic modulus in micron-scale spatial resolution and their applications in rapid collection of composition-phase-property data.

Beyond characterization, Materials Engineering and Materials Science are concerned with prediction and explanation of properties, from a structural standpoint. Two articles were chosen to highlight important considerations when making this connection. The article by Lewis, Qidwai, Geltmacher, and Jackson highlight the actual details of turning a 3-D characterization into property predictions. We take it for granted what a microstructure is, but the actual definition of a microstructure must be a statistical one, whose true description is currently an active area of research. The article by McDowell, Ghosh, and Kalidindi describes the current state of the art of representing random media for the purposes of modeling properties in Materials Science and Engineering.

The increasing data rate of modern microscopy is generating a new focus for research: that of converting measurements to context. The output of a microscope observation is typically an image that the eye can interpret, if sufficient care is taken. Microstructure images actually consist of thousands or millions of individual measurements that the eye interprets. The actual value stored in each pixel was the magnitude of a measurement. For this reason, image data is often referred to as a memory-based representation. Converting this to a Materials context-based representation required by the physics-based models used to compute properties constitutes an emerging problem in large dataset generation: that of analysis.

The article by Rowenhorst presents a comprehensive description of the issues involved in converting 3-D serial section data to a Materials context. Since this is a painstaking process, research is being devoted towards developing algorithms that require less human interaction to analyze the datasets. The field of image segmentation is an exploding field, mostly fueled by the proliferation of medical imagery and the introduction of the digital camera: it is not possible to cover this field with any fidelity. Instead, we have chosen to highlight several techniques currently in development for performing segmentations in Materials images. The articles by Bouman and Comer, Pollak, Wang and Waggoner, and by Shiflet describe four promising techniques: (1) statistical segmentation, including Bayesian methods, (2) inverse diffusion, (3) graph-cut methods, and (4) level set methods, respectively.

The articles covered in this issue represent only a sampling of the exciting developments in this rapidly expanding field. It is with regrets that we could not cover all of the interesting developments in the field, including 3D Atom Probe, MultiModal data collection and Fusion, 3-D + t time series tomography, the many physics based "forward models" that can be validated for the first time with the rich datasets being collected, among many others. Watch this space for further developments.

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